

# hydrogen atom: center-of-mass and relative

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2-particle problem (electron & proton)

$$\left[ -\frac{\hbar^2}{2m_e} \Delta_e - \frac{\hbar^2}{2m_p} \Delta_p + V(|\vec{r}_e - \vec{r}_p|) \right] \Psi(\vec{r}_e, \vec{r}_p) = E \Psi(\vec{r}_e, \vec{r}_p)$$

separation in center-of-mass and relative coordinates

$$\vec{R} = \frac{m_e \vec{r}_e + m_p \vec{r}_p}{m_e + m_p}$$

$$M = m_e + m_p$$

$$\vec{r} = \vec{r}_e - \vec{r}_p$$

$$\mu = \frac{m_e m_p}{m_e + m_p}$$

$$-\frac{\hbar^2}{2M} \Delta_R S(\vec{R}) = E_{\text{CM}} S(\vec{R}) \quad \left[ -\frac{\hbar^2}{2\mu} \Delta_r + V(|\vec{r}|) \right] \psi(\vec{r}) = E_H \psi(\vec{r})$$

$$\Psi(\vec{r}_e, \vec{r}_p) = S(\vec{R}) \psi(\vec{r}) \quad \text{and} \quad E = E_{\text{CM}} + E_H$$

# hydrogen atom: spherical separation

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relative motion

$$\left[ -\frac{\hbar^2}{2\mu} \Delta_r + V(|\vec{r}|) \right] \psi(\vec{r}) = E_H \psi(\vec{r})$$

spherical symmetry

$$\psi(\vec{r}) = \frac{u(r)}{r} Y_{l,m}(\theta, \phi)$$

$$\left( -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu} \frac{l(l+1)}{r^2} - \frac{e^2}{4\pi\epsilon_0 r} \right) u(r) = E_H u(r)$$

dimensionless units:  $\rho = \kappa r$  with  $\kappa^2 = 2m|E|/\hbar^2$  and  $\rho_0 = 2me^2 / (4\pi\epsilon_0 \hbar^2 \kappa)$

$$\left( \frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{\rho_0}{\rho} - 1 \right) u(\rho) = 0$$

# hydrogen atom: radial solution

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ansatz (solve asymptotics)

$$u(\rho) = \rho^{l+1} w(\rho) e^{-\rho}$$

differential equation for  $L(s)$ :

$$\rho \frac{d^2 w}{d\rho^2} + 2(l+1-\rho) \frac{dw}{d\rho} + (\rho_0 - 2(l+1))w = 0$$

ansatz: power series

$$w(\rho) = \sum_{k=0}^{\infty} a_k \rho^k$$

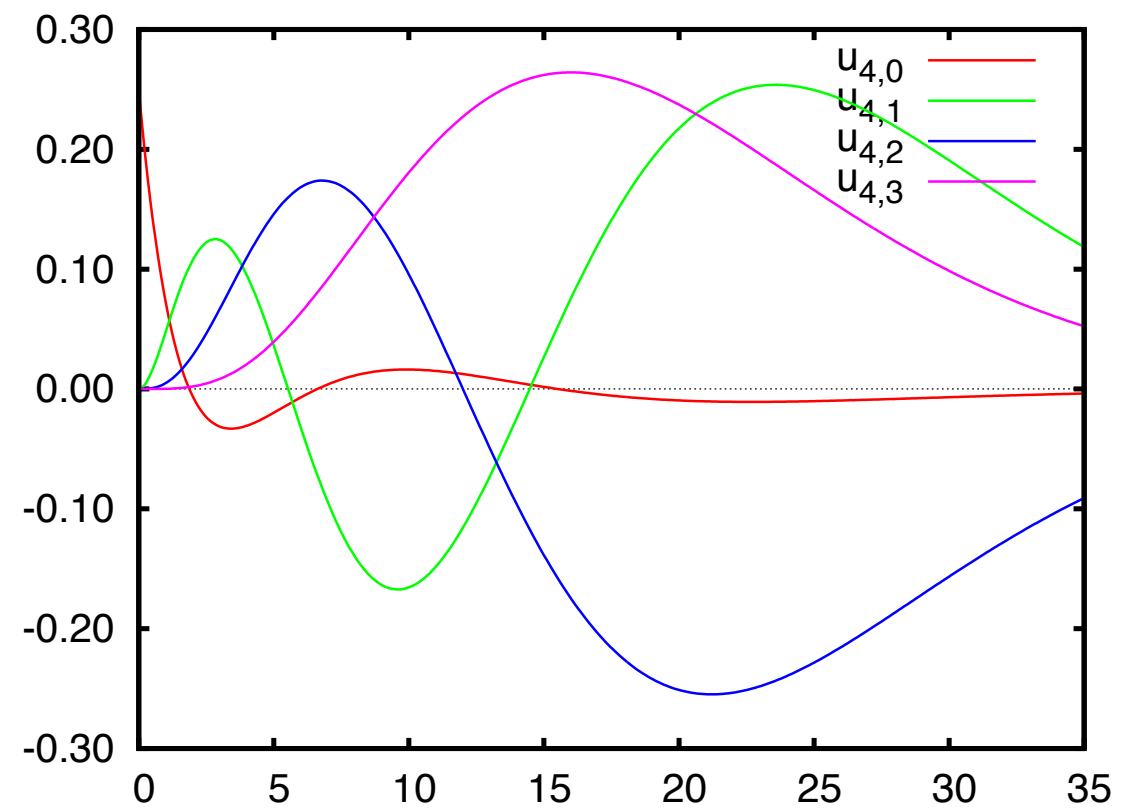
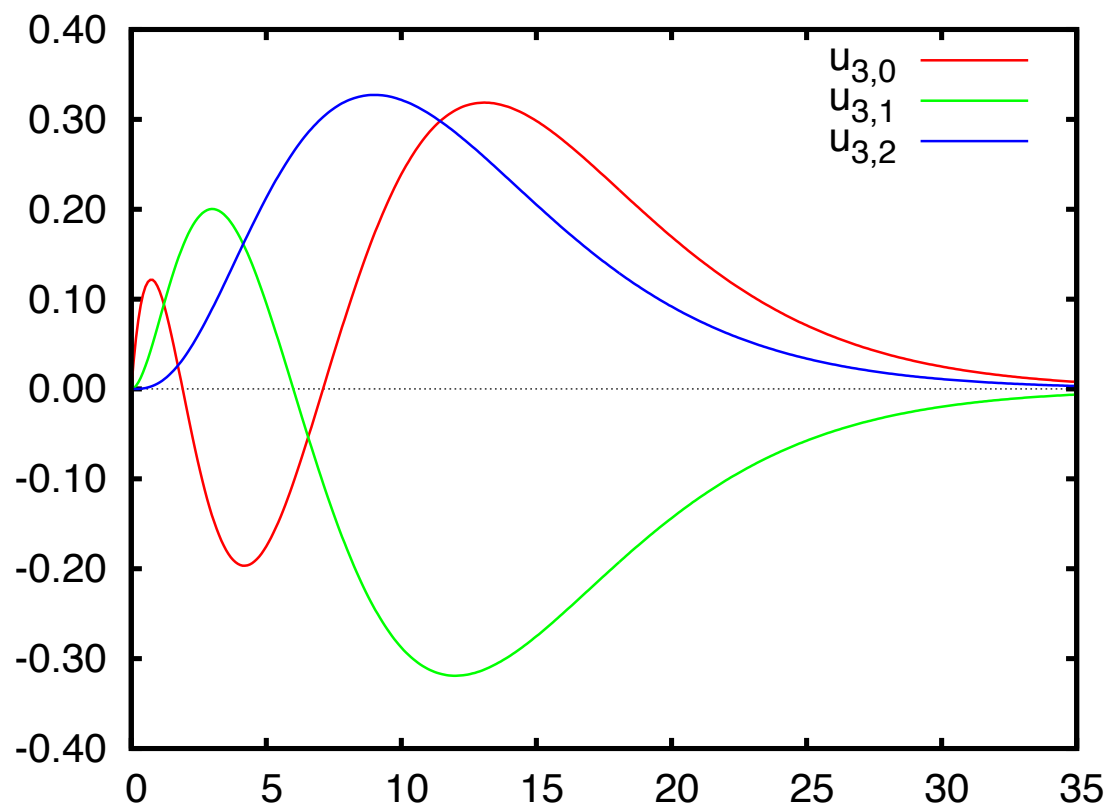
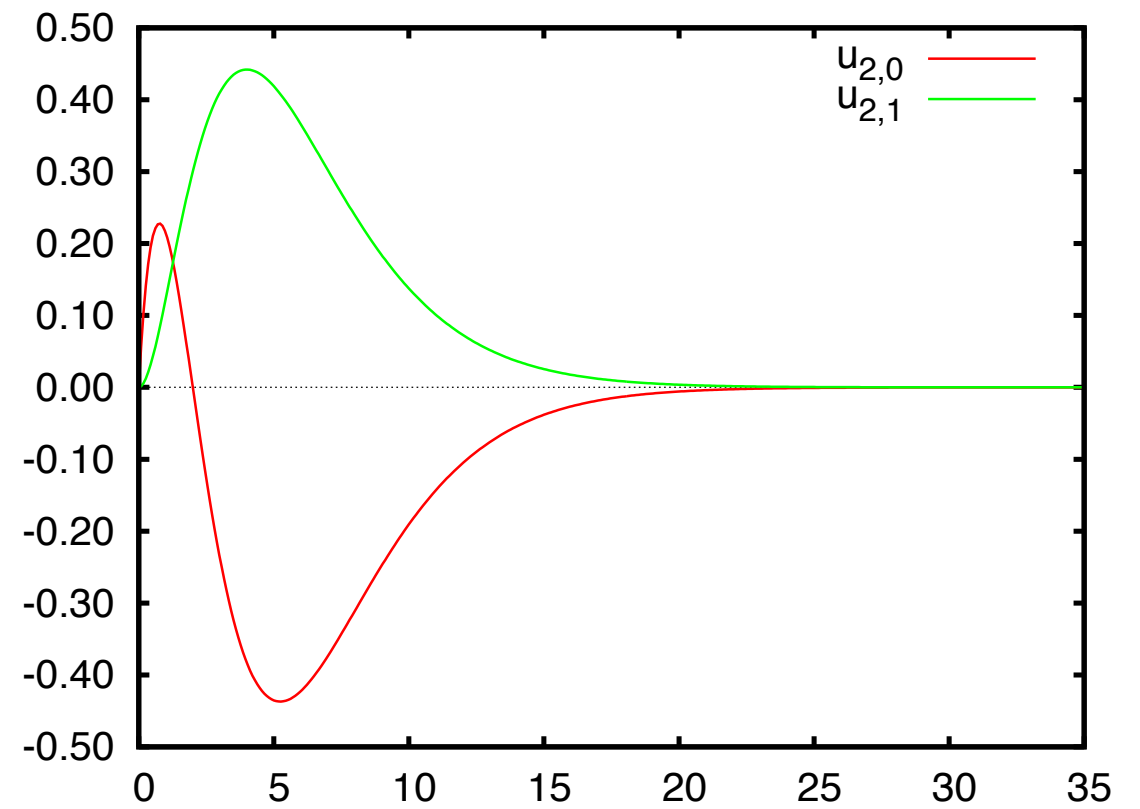
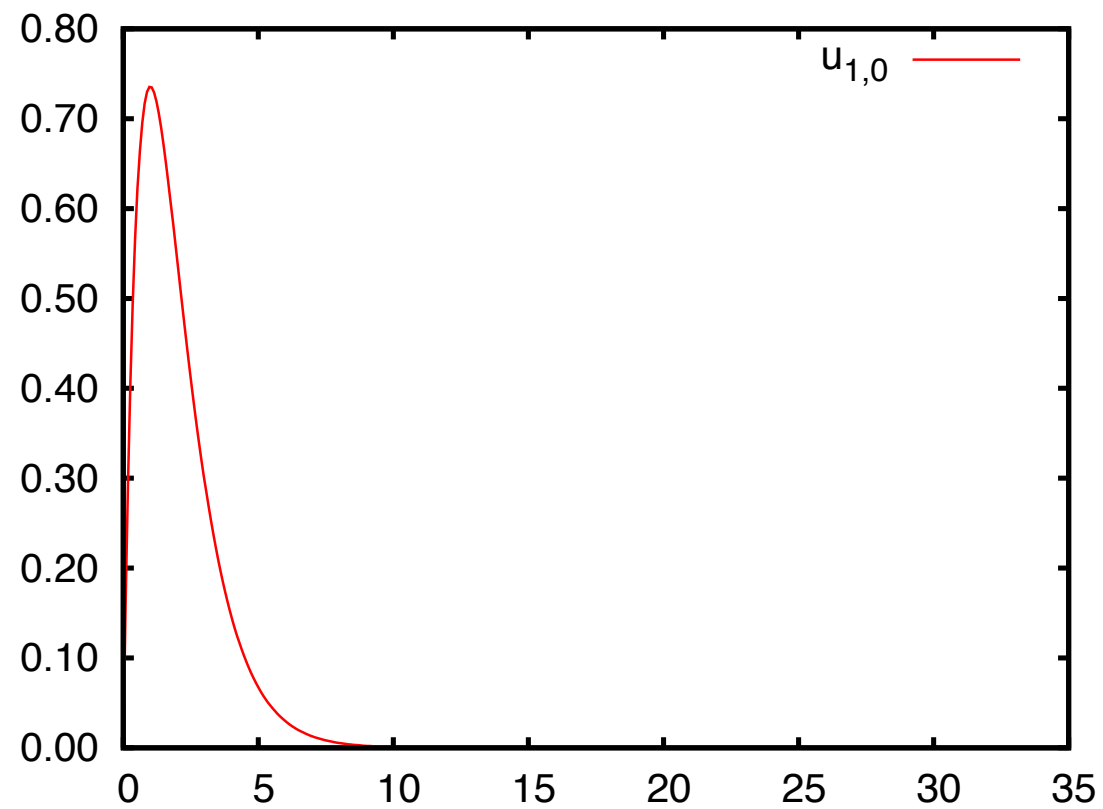
recursion for coefficients

$$a_{k+1} = -\frac{2(k+l+1) - \rho_0}{(k+1)(k+2l+2)} a_k$$

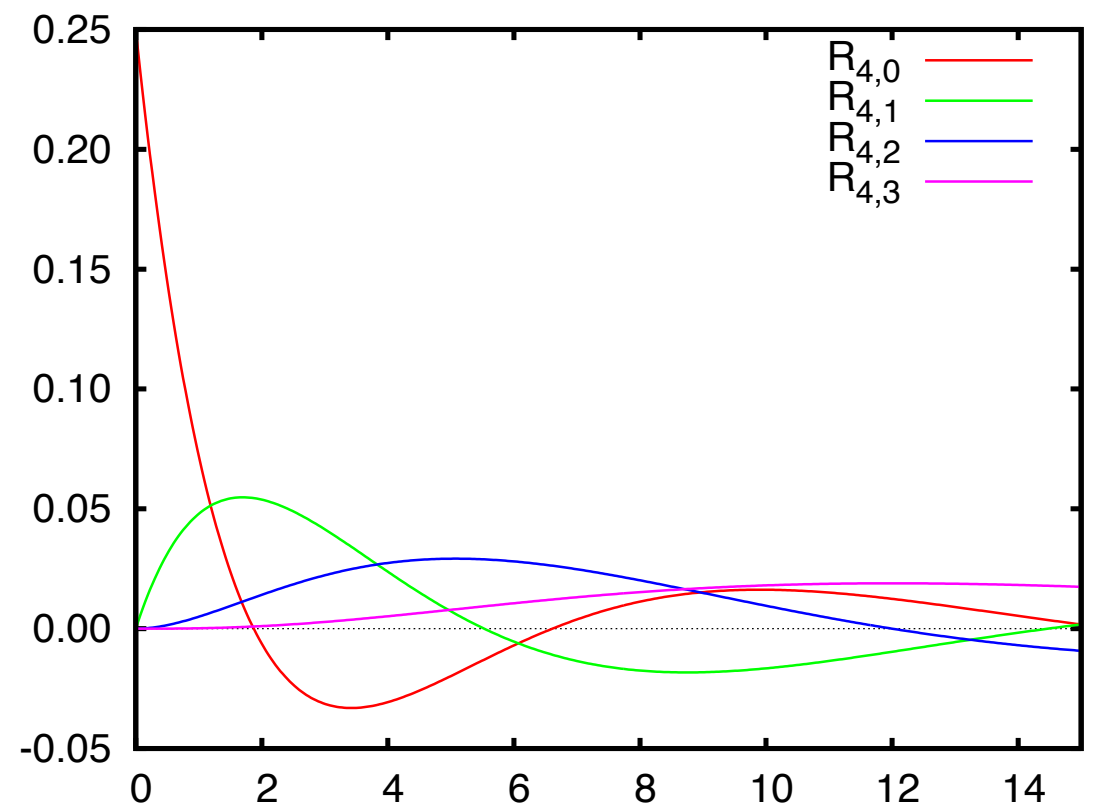
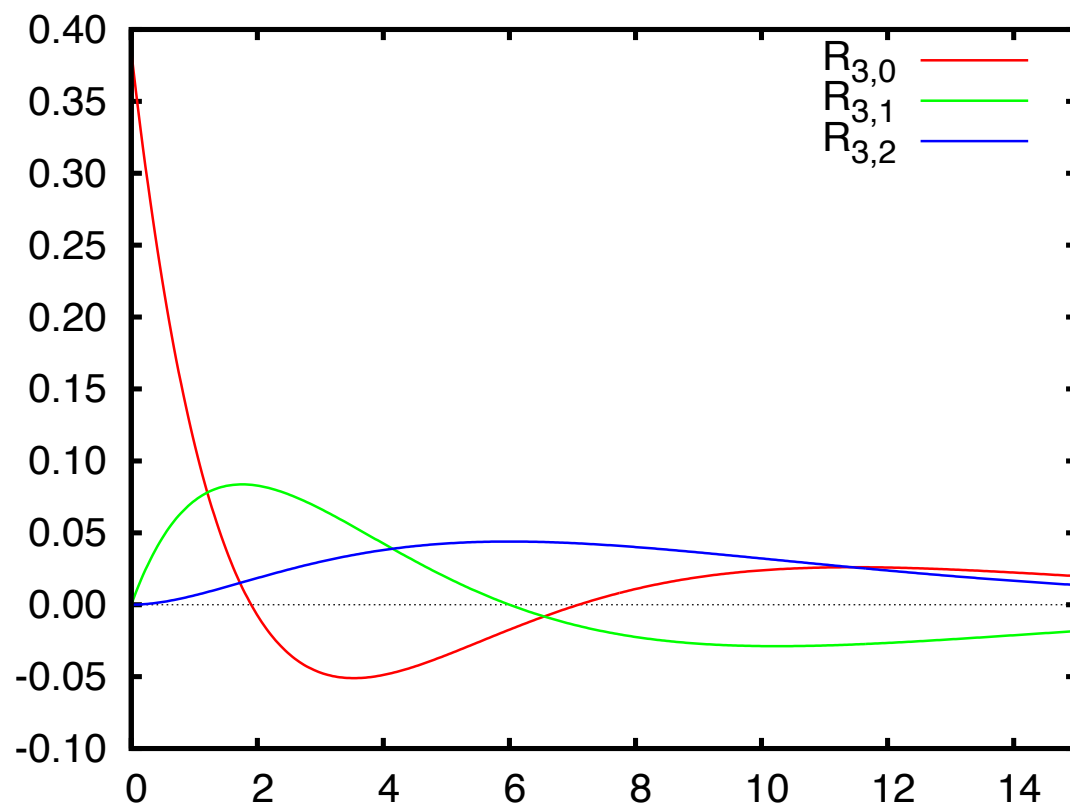
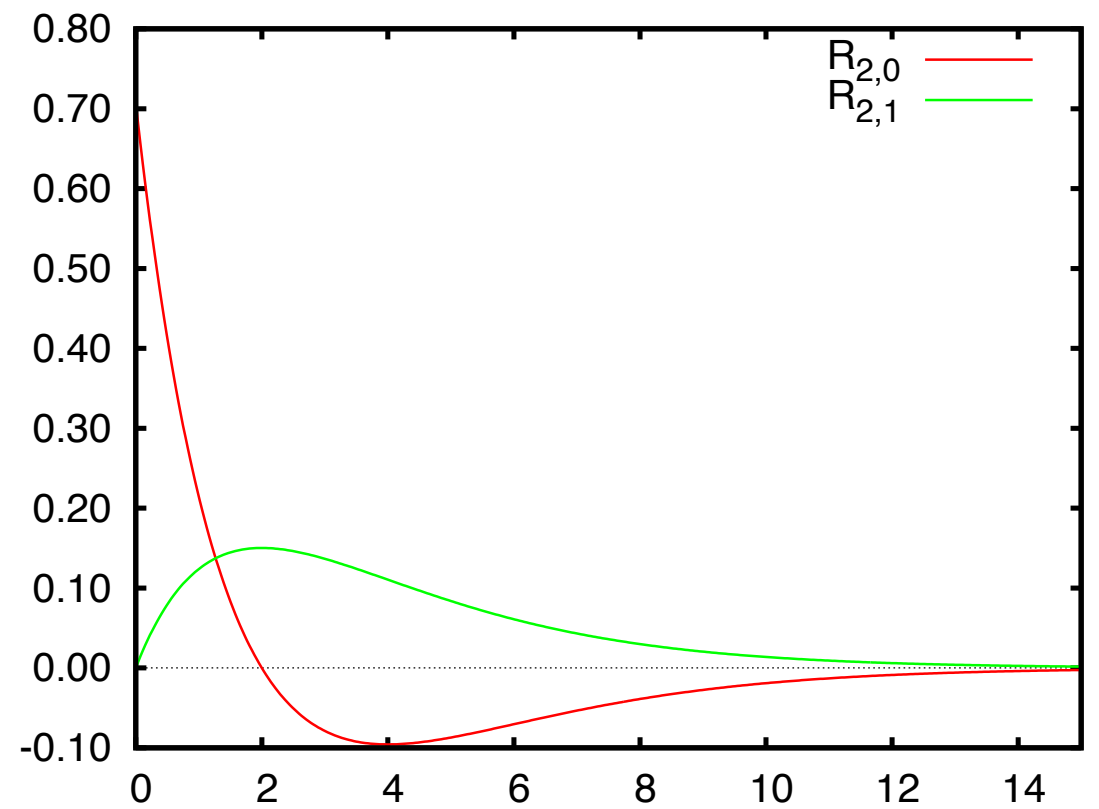
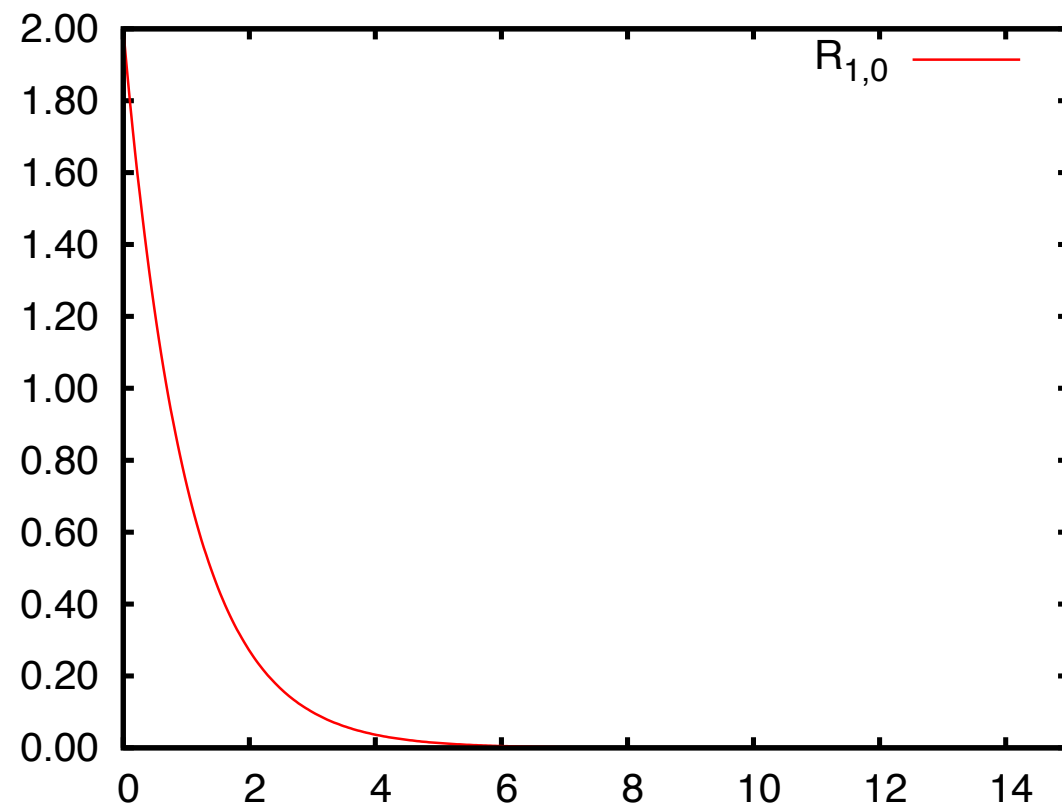
normalizability: recurrence must terminate at some finite  $k$

$$n \geq l+1$$

# radial functions $u_{nl}(r) = r R_{nl}(r)$



# radial functions $R_{nl}(r)$



A simplified periodic table diagram. It consists of several blocks of colored squares. On the far left, there is a yellow block of 10 squares arranged in two columns of five. To its right is a green block of 10 squares in a single row. Further right is a red block of 10 squares in a single row. To the right of the red block is a blue block of 10 squares arranged in two columns of five. Finally, on the far right, there is a single yellow square.

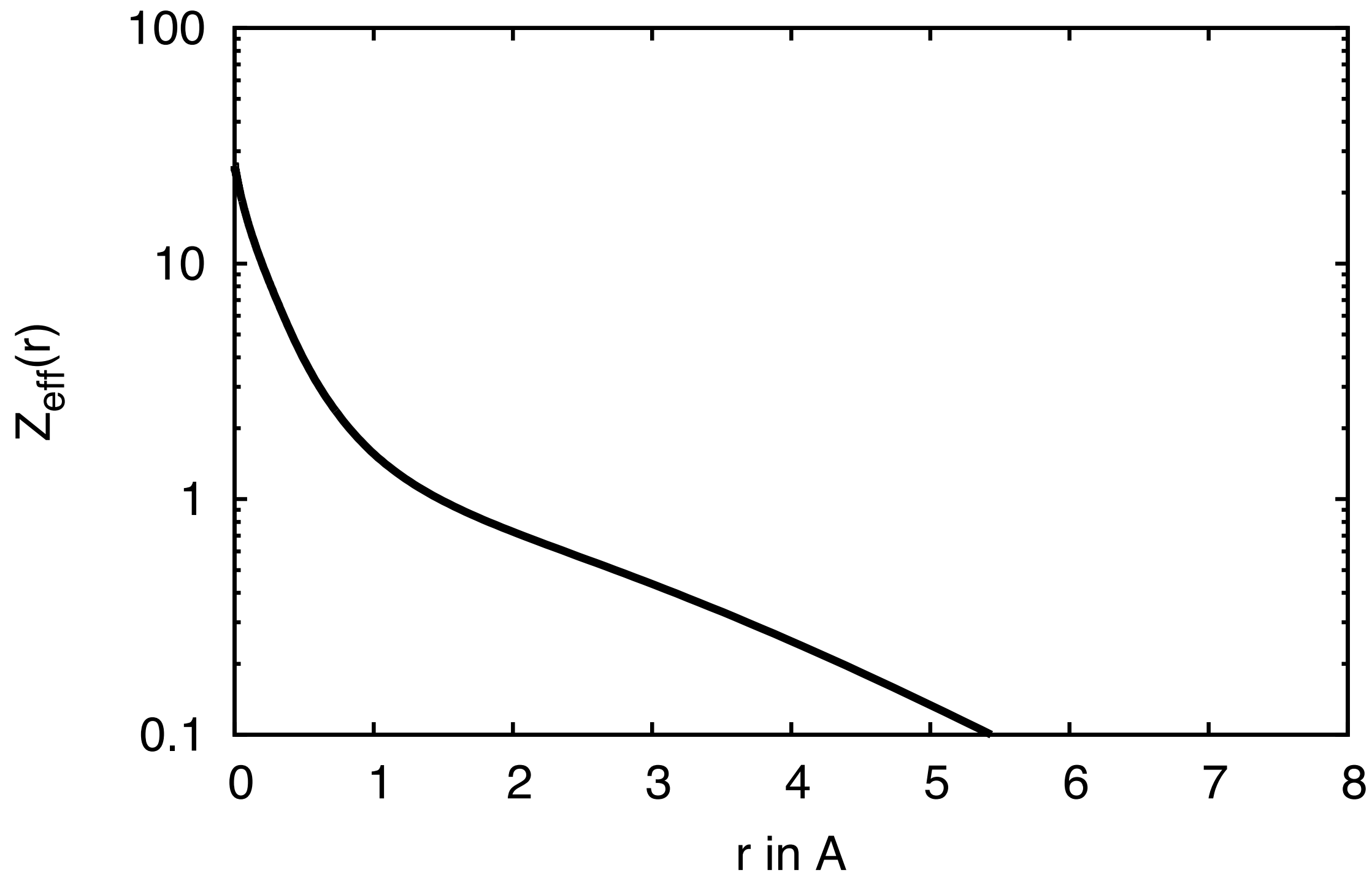
The diagram illustrates the relative sizes and shapes of atomic orbitals for principal quantum numbers  $n = 1$  through  $n = 7$ . The orbitals are color-coded: yellow for s, blue for p, red for d, and green for f. The orbitals are arranged in a grid, with the principal quantum number  $n$  indicated on the left and the orbital type indicated on the right. The orbitals are shown as concentric shells, with the size increasing significantly with  $n$ . The s orbitals are spherical, p orbitals are dumbbell-shaped, d orbitals are cloverleaf-shaped, and f orbitals are complex. The diagram shows that the size of the orbitals increases rapidly with  $n$ , and the number of orbitals of a given type increases with  $n$ .

$n$	s	p	d	f
1	1s			
2	2s	2p		
3	3s	3p	3d	
4	4s	4p	4d	4f
5	5s	5p	5d	5f
6	6s	6p	6d	
7	7s			

# atom in spherical mean-field approximation

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Fe : [Ar] 3d<sup>6</sup> 4s<sup>2</sup> 4p<sup>0</sup>



# Atom- und Hybrid-Orbitale

